

APPENDIX 1

Program for Baselineing, Normalizing, Interpolating Then Calculating Spectral Overlap Integrals

```
5      C      This program has a non-standard DO WHILE loop

      INTEGER NPTS, NMAX, ROWS, ITER
      INTEGER EOF1, FLERR1, FLERR2
      INTEGER EOF2, FLERR3, FLERR4
10     INTEGER EOF3, FLERR5, FLERR6
      INTEGER FLERR7
      INTEGER i,j
      CHARACTER*30 fname1, fname2, fname3, fname4
      CHARACTER*30 fname5, fname6, fname7
15     PARAMETER(NMAX=3500, LAMDA=601)
      REAL x,xx1 (NMAX) ,yy1 (NMAX),INTERV1
      REAL xx2 (NMAX) ,yy2 (NMAX), INTERV2

      REAL xx3 (NMAX), yy3 (NMAX),INTERV3
20     REAL yil (NMAX), yi2 (NMAX), yi3 (NMAX), yc (NMAX)
      REAL area
      CHARACTER*1 SUBSTR, INITAR, LIGHT, INTMED

      FLERR1=0
25     FLERR2=0
      FLERR3=0
      FLERR4=0
      FLERR5=0
      FLERR6=0
30     FLERR7=0
      EOF1=0
      EOF2=0
      EOF3=0
      INTERV1=0
35     INTERV2=0
      INTERV3=0
      area=0

      write(*,*) 'Do you wish to output intermediate files? (Y/N)'
40     read(*,'(A)') INTMED

      write(*,*) 'Do you wish to process a substrate file? (Y/N)'
      read(*,'(A)') SUBSTR

45     IF ((SUBSTR.EQ.'Y') .OR. (SUBSTR.EQ.'y')) THEN
```

```

ITER=0
do 5 ITER=1, NMAX
    xx1 (ITER)=0
    yy1 (ITER)=0
    yi1 (ITER)=0
5    continue

write(*,*) 'Enter the name of the input substrate file:'
10 read(*,' (A)') fname1

open
(UNIT=11,FILE=fname1,STATUS='OLD',IOSTAT=FLERR1,E
RR=101)
15

ROWS=0

do while ((EOF1.EQ.0) .AND. (ROWS.LT.NMAX))
    ROWS=ROWS+1
    Read (11,*,IOSTAT=EOF1) xx1 (ROWS), yy1 (ROWS)
end do

close (UNIT=11)
NPTS=0

25 IF (EOF1.NE.0) THEN
    NPTS=ROWS-1
    write(*,'(I4,1X,A12)') NPTS, 'points read.'
ELSE
    NPTS=ROWS
    write(*,'(A28, I4, A12)') 'Too many data points! First',
+                               NMAX,' points read...'
30 END IF

35 call baseIn(yy1,NPTS)

IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

    write(*,*) 'Enter the name of the output substrate file:'
40 read(*,' (A)') fname2
    open
(UNIT=12,FILE=fname2,STATUS='NEW',IOSTAT=FLERR2,
ERR=102)

45 write(*,*) 'Writing data...'

END IF

```

```

x=0
i=0
j=0
5
do 12 i=1, LAMDA

    x= (i-1)+200

10    call locate(xx1,NPTS,x,j)

    if ((j.eq.0). OR. (j.eq.NPTS)) then
        INTERV1=0
    else
15        INTERV1= ((yyl(j+1)-yyl(j)) / (xx1(j+1) - xx1(j))) *
        (x-xx1(j))
        +          +yyl(j)

    end if
20    yi1 (i)=INTERV1

    IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

25        if ((j.eq.0) .OR. (j.eq.NPTS)) then
            GO TO 12
        else
            write(12,'(1x, f7.2,i6,3f12.2)')x,j,xx1(j),xx1(j+1),
+            INTERV1
30            endif

        END IF

35        12          continue
        IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
            close (UNIT=12)

        END IF

40        ELSE
            ITER=0
            do 14 ITER=1, LAMDA
                yi1 (ITER) =1
45        14          continue

        ENDIF

```

```

write(*,*) 'Do you wish to process an initiator file? (Y/N)'
read(*,'(A)') INITAR

5      IF ((INITAR.EQ.'Y') .OR. (INITAR.EQ.'y')) THEN

            ITER=0

do 15 ITER=1,NMAX
10      xx2 (ITER) =0
            yy2 (ITER) =0
            yi2 (ITER) =0
15      continue

15      write(*,*) 'Enter the name of the initiator file:'
read(*,'(A)') fname3

open
(UNIT=13,FILE=fname3,STATUS='OLD',IOSTAT=FLERR3,
20      ERR=103)

ROWS=0

do while ((EOF2.EQ.0) .AND. (ROWS.LT.NMAX))
25      ROWS=ROWS+1
            read(13,*,IOSTAT=EOF2) xx2 (ROWS), yy2 (ROWS)
end do

close (UNIT=13)

30      NPTS=0

IF (EOF2.NE.0) THEN
            NPTS=ROWS-1
35      write(*,1(14,1X,A12)) NPTS,'points read.'
ELSE
            NPTS=ROWS
            write (*,'(A28,I4,A12)') 'Too many data points! First ',
+
40      NMAX,' points read...'
            END IF
            call baseln (yy2,NPTS)

IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

45      write(*,*) 'Enter the name of the output initiator file: '
read(*,'(A)') fname4

```

```

      open
      (UNIT=14,FILE=fname4,STATUS='NEW',IOSTAT=FLERR4,
      ERR=104)

```

```

5          write(*,*) 'Writing data...'

```

```

      END IF

```

```

      x=0

```

```

      i=0

```

```

10      j=0

```

```

      do 22 i=1,LAMDA
          x= (i-1)+200

```

```

15          call locate (xx2,NPTS,x,j)

```

```

      if ((j.eq.0).OR. (j.eq.NPTS)) then

```

```

          INTERV2=0

```

```

      else

```

```

20          INTERV2= ((yy2(j+1)-yy2(j)) / (xx2(j+1) - xx2
      (j))) * (x-xx2 (j))
      +
          +yy2 (j)

```

```

      end if

```

```

      yi2 (i)=INTERV2

```

```

25      IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

```

```

          if ((j.eq.0) .OR. (j.eq.NPTS)) then

```

```

              GO TO 22

```

```

          else

```

```

30          write(14,'(1x,f7.2,i6,3f12.2)') x, j, xx2
      (j),xx2 (j+1),
      +

```

```

          INTERV2

```

```

      endif

```

```

35      END IF

```

```

22      continue

```

```

40      IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

```

```

          close (UNIT=14)

```

```

      END IF

```

```

      ELSE

```

```

45      ITER=0

```

```

do 24 ITER=1,LAMDA
    yi2 (ITER)=1
24    continue

5    ENDIF
    write(*,*) 'Do you wish to process a light source file? (Y/N)'
    read(*,'(A)') LIGHT

    IF ((LIGHT.EQ.'Y').OR. (LIGHT.EQ.'y')) THEN
10        ITER=0
        do 25 ITER=1,NMAX
            xx3 (ITER) =0
            yy3 (ITER) =0
            yi3 (ITER)=0
15        25    continue

        write(*,*) 'Enter the name of the light source file:'
        read(*,'(A)') fname5

20        open
        (UNIT=15,FILE=fname5,STATUS='OLD',IOSTAT=FLERR5,
        ERR=105)

        ROWS=0

25        do while ((EOF3.EQ.0) .AND. (ROWS.LT.NMAX))
            ROWS=ROWS+1
            read(15,*,IOSTAT=EOF3) xx3 (ROWS), yy3 (ROWS)
        end do

30        close (UNIT=15)

        NPTS=0
        IF (EOF3.NE.0) THEN
35            NPTS=ROWS-1
            write(*,1 (14,1X,A12)1) NPTS, 'points read.'
        ELSE
            NPTS=ROWS
            write (*,'(A28,I4,A12)') 'Too many data points! First ',
40            +                NMAX,' points read...'
            END IF

            call norm (yy3,NPTS)

45        IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

            write(*,*) 'Enter the name of the light source output file:'

```

```

        read(*,' (A)') fname6
        open
        (UNIT=16,FILE=fname6,STATUS='NEW',IOSTAT=FLERR6,
5         ERR=106)

```

```

        write(*,*) 'Writing data...'

```

```

    END IF

```

```

    x=0

```

```

    i=0

```

```

    j=0

```

```

    do 32 i=1,LAMDA

```

```

        x= (i-1)+200

```

```

        call locate (xx3,NPTS,x,j)

```

```

        if ((j.eq.0) .OR. (j.eq.NPTS)) then

```

```

            INTERV3=0

```

```

        else

```

```

            INTERV3= ((yy3(j+1) - yy3(j)) / (xx3(j+1) -
20      xx3(j))) * (x-xx3 (j))

```

```

            +
                +yy3 (j)

```

```

        end if

```

```

        yi3 (i) =INTERV3

```

```

        IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

```

```

            if ((j.eq.0).OR. (j.eq.NPTS)) then

```

```

                GO TO 32

```

```

            else

```

```

                write(16,'(1x,f7.2,i6,3f12.2)') x,j,xx3 (j),xx3 (j+1),
30      +
                    INTERV3

```

```

            endif

```

```

    END IF

```

```

35      32      continue

```

```

    IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

```

```

        close (UNIT=16)

```

```

    END IF

```

```

    ELSE

```

```

    ITER=0

```

```

45      do 34 ITER=1,LAMDA

```

```

        yi3 (ITER) -1

```

```

34      continue

```

ENDIF

ITER=0

DO 40 ITER=1,LAMDA

yc (ITER)=0

40 CONTINUE

DO 55 i=1,LAMDA

yc (i) =yi1 (i)*yi2 (i)*yi3 (i)

55 CONTINUE

write(*,*) 'Enter the filename for cumulative data:'

read (*, '(A)') fname7

open

(UNIT=17,FILE=fname7,STATUS='NEW',IOSTAT=FLERR7,
ERR=107)

write(*,*) 'Writing data...'

CALL integ (yc,LAMDA,area)

write(*, '(1X,A26,A11,F12.6)') 'The area under the product',
+'curve is:',area

write(17, '(1X,A26,A11,F12.6)') 'The area under the product',
+' curve is: ',area

DO 60 i=1,LAMDA

x= (i-1)+200

write(17, '(1X,F6.1,2F11.2,F11.4,E15.6)') x,yi1 (i),yi2

(i),

+ yi3 (i) ,yc (i)

60 CONTINUE

close (UNIT=17)

101 IF (FLERR1 .NE. 0) THEN

write(*,*) 'Unable to open substrate file!'

END IF

102 IF (FLERR2 .NE. 0) THEN

write(*,*) 'Unable to create substrate output file!'

END IF

103 IF (FLERR3 .NE. 0) THEN

write(*,*) 'Unable to open initiator file!'

END IF

104 IF (FLERR4 .NE. 0) THEN
write(*,*) 'Unable to create initiator output file!'
END IF

105 IF (FLERR6 .NE. 0) THEN
write(*,*) 'Unable to open light source file!'
END IF

106 IF (FLERR6 .NE. 0) THEN
write(*,*) 'Unable to create light source output file!'
END IF

107 IF (FLERR7 .NE. 0) THEN
write(*,*) 'Unable to create cumulative output file!'
END IF

write(*,*) 'Program exiting normally...'

END

SUBROUTINE locate (xx,n,x,j)

INTEGER j,n

REAL x,xx (n)

INTEGER j1,jm,ju

J1=0

ju=n+1

10 if (ju-j1.gt.1) then

jm= (ju+j1) /2

if ((xx (n).ge.xx (1)) .eqv. (x.ge.xx (jm))) then

j1=j m

else

ju=jm

endif

goto 10

endif

if (x.eq.xx (1))then

j=1

else if (x.eq.xx(n))then

j=n-1

else

j=j1

endif

return END

SUBROUTINE baseln (yy,N)

INTEGER N, i
REAL yy (N), minno, temp

minno=yy (1)
i=0
temp=0

DO 10 i=2,N
IF (yy (i) .LT. minno) THEN
minno=yy (i)
END IF
CONTINUE

i=0

DO 20 i=1,N
temp=yy (i)-minno
yy (i)=temp
CONTINUE

END

SUBROUTINE norm (yy,N)

INTEGER N, i
REAL yy (N),maxno,temp

maxno=yy (1)
i=0
temp=0

DO 5 i=2,N
IF (yy(i).GT.maxno) THEN
maxno=yy (i)
END IF
CONTINUE

i=0

DO 10, i=1,N
temp=yy (i)/maxno
yy (i)=temp
CONTINUE

END

SUBROUTINE integ (yy,N,area)

INTEGER N,i

REAL yy (N),sum,area

i=0

sum=0

area=0

DO 10 i=1,N-1

sum=sum+ (yy(i)+yy (i+1))*0.5

10 CONTINUE

area=sum/100000

END

APPENDIX 2

Program to create uniformly spaced csv data from unevenly spaced
tabular data

```
5      #include <stdio.h>
      #include <stdlib.h>
      #include <math.h>

10     #define NMAX 3501
      #define STRMAX 151
      #define FNMAX 81
      #define OUTPTS 801

15     void locate(float xx[], unsigned long n, float x, unsigned long *j);
      void norm(float xx[], unsigned long int n);
      void baseline(float xx[], unsigned long int n);

20     int main()
      {
      char fnamein(FNMAX], string[STRMAX], *str, ptr,
      fnameout[FNMAX], another;
      float xdata(NMAX], ydata[NMAX], xinter[OUTPTS+1],
      yinter[OUTPTS+1];
25     unsigned long int index, i, j;
      int choice;
      FILE *fpin, *fpout;

      another = 'Y';

30     do {
          for (i = 0; i <= NMAX-1; i++) {
              xdata [i] = 0;
              ydata [i] = 0;

35     };

          for (i = 0; i <= OUTPTS; i++) {
              xinter [i] = 0;
              yinter (i] = 0;

40     };

      printf("Enter name of the input file (80 chars max, no spaces): ");
      scanf("%s", fnamein);

45     printf("File name is %s\n",fnamein);

      fpin = fopen(fnamein,"r");

      if (fpin == NULL) {
```

```

    printf("Cannot open %s\n",fnamein);
    exit(1);
};

5    index = 1;

    while (1) {
        str_ptr = fgets(string,STRMAX-1,fpin);
        if(str_ptr == NULL)
10         break;
        if (index == NMAX)
            break;
        sscanf (string, "%f %f" , &xdata [index] , &ydata [index]);
        index++;
15    };

```

```

f close (fpin);

if((index == NMAX) && (str_ptr != NULL)) {
    index--;
    printf("Too many data points! Using first %d points
20    only...\n",index);
}
else {
    index--;
    printf("%d points read...\n",index);
};
25

```

```

printf("\nEnter option for data processing\n");
printf("1: Normalize the data after interpolation\n");
printf("2: Baseline the data after interpolation\n");
printf("3: First interpolate, then baseline and finally ");
printf("normalize the data\n");
printf("4: Simply interpolate the data\n");
35 printf("5: Simply normalize the data\n");
printf("6: Simply baseline the data\n");
printf("or\n");
printf("0: to exit the program without any data processing\n");
printf("\nEnter option (0-6): ");
40 scanf("%d",&choice);

```

```

if (choice == 0)
    exit(2);

```

```

45 printf("\nEnter name of the output file (80 chars max, no spaces): ");
scanf("%s",fnameout);

```

```

printf("File name is %s\n",fnameout);

```

```

fpout = fopen(fnameout,"w");

if (fpout == NULL) {
    printf("Cannot open %s\n",fnameout);
    exit(3);
};

for(i = 1; i <= OUTPTS; i++) {
    xinter[i] = 200+((float)i-1);
    locate(xdata,index,xinter[i],&j);
    if ((j == 0) || (j == index))
        yinter[i] = 0;
    else
        yinter[i] = (xinter[i] - xdata[j]) * ((ydata[j+1] - ydata[j]) /
            (xdata[j+1] - xdata[j])) + ydata[j];
};

if ((choice == 2) || (choice == 3)) {
    baseline(yinter,OUTPTS);
};

if (choice == 6) {
    baseline(ydata,index);
};

if ((choice == 1) || (choice == 3)) {
    norm(yinter,OUTPTS);
};

if (choice == 5) {
    norm(ydata,index);
};

if ((choice >= 1) && (choice <= 4)) {
    for (i = 1; i <= OUTPTS-1; i++) {
        fprintf(fpout,"%13.5E, ",yinter[i]);
    };
    fprintf(fpout,"%13.5E\n",yinter[OUTPTS]);
}
else
    if ((choice == 5) || (choice == 6)) {
        for (i = 1; i <= index-1; i++)
            fprintf(fpout,"%13.5E, ",ydata[i]);
        };
        fprintf(fpout,"%13.5E\n",ydata[index]);
    };

fclose(fpout);

```

```

    printf("File %s written.\n\n",fnameout);
    printf("Process another file (Y/y/N/n)? : ");
    scanf("%ls",&another);
} while (another == 'Y' || another == 'y');

```

```

printf("Exiting...\n");
return(0);
}

```

```

void locate(float xx[], unsigned long n, float x, unsigned long *j)
{
    unsigned long ju,jm,jl;
    int ascnd;

```

```

    jl=0;
    ju=n+1;
    ascnd=(xx[n] >= xx[1]);
    while (ju-jl > 1) {
        jm=(ju+jl) >> 1;
        if (x >= xx[jm] == ascnd)
            jl=jm;
        else
            ju=jm;
    }
    if (x == xx[1])
        *j=1;
    else if (x == xx[n])
        *j=n-1;
    else
        *j=jl;
}

```

```

void norm(float xx[], unsigned long int n)
{
    unsigned long int i;
    float maxdata, temp;

    maxdata = xx[1];
    temp = 0;

    for(i = 2; i <= n; i++) {
        if(xx[i] > maxdata)
            maxdata = xx[i];
    };

    for(i = 1; i <= n; i++) {
        temp = xx[i]/maxdata;
        xx[i] = temp;
    };
}

```

Parameter	Value	Unit
Temperature	25.0	°C
Pressure	1.0	atm
Humidity	50.0	%
Light intensity	100.0	μmol photons m ⁻² s ⁻¹
CO ₂ concentration	400.0	ppm
Water potential	-0.1	MPa
Root length	10.0	cm
Stomatal conductance	0.1	mol m ⁻² s ⁻¹
Photosynthetic rate	1.0	μmol CO ₂ m ⁻² s ⁻¹
Transpiration rate	1.0	mmol H ₂ O m ⁻² s ⁻¹
Chlorophyll content	10.0	mg g ⁻¹
Protein content	1.0	mg g ⁻¹
Carbohydrate content	1.0	mg g ⁻¹
Antioxidant activity	1.0	μg g ⁻¹
Cell wall thickness	1.0	μm
Membrane integrity	1.0	μm
Gene expression	1.0	fold
Protein synthesis	1.0	fold
Enzyme activity	1.0	fold
Signal transduction	1.0	fold
Cell cycle	1.0	fold
Apoptosis	1.0	fold
Autophagy	1.0	fold
Mitochondrial function	1.0	fold
Chloroplast function	1.0	fold
Endoplasmic reticulum	1.0	fold
Golgi apparatus	1.0	fold
Lysosome	1.0	fold
Vacuole	1.0	fold
Nucleus	1.0	fold
Cytoplasm	1.0	fold
Plasma membrane	1.0	fold
Cell wall	1.0	fold
Extracellular matrix	1.0	fold
Intercellular space	1.0	fold
Soil	1.0	fold
Atmosphere	1.0	fold
Water	1.0	fold
Light	1.0	fold
CO ₂	1.0	fold
Temperature	1.0	fold
Humidity	1.0	fold
Pressure	1.0	fold
Gravity	1.0	fold
Magnetic field	1.0	fold
Electric field	1.0	fold
Sound	1.0	fold
Vibration	1.0	fold
Shock	1.0	fold
Stress	1.0	fold
Damage	1.0	fold
Recovery	1.0	fold
Adaptation	1.0	fold
Evolution	1.0	fold
Speciation	1.0	fold
Extinction	1.0	fold
Conservation	1.0	fold
Management	1.0	fold
Policy	1.0	fold
Law	1.0	fold
Ethics	1.0	fold
Society	1.0	fold
Culture	1.0	fold
Religion	1.0	fold
Philosophy	1.0	fold
Art	1.0	fold
Literature	1.0	fold
Science	1.0	fold
Technology	1.0	fold
Industry	1.0	fold
Commerce	1.0	fold
Finance	1.0	fold
Health	1.0	fold
Education	1.0	fold
Government	1.0	fold
Law	1.0	fold
Justice	1.0	fold
Peace	1.0	fold
War	1.0	fold
Conflict	1.0	fold
Cooperation	1.0	fold
Competition	1.0	fold
Collaboration	1.0	fold
Partnership	1.0	fold
Relationship	1.0	fold
Community	1.0	fold
Society	1.0	fold
Culture	1.0	fold
Religion	1.0	fold
Philosophy	1.0	fold
Art	1.0	fold
Literature	1.0	fold
Science	1.0	fold
Technology	1.0	fold
Industry	1.0	fold
Commerce	1.0	fold
Finance	1.0	fold
Health	1.0	fold
Education	1.0	fold
Government	1.0	fold
Law	1.0	fold
Justice	1.0	fold
Peace	1.0	fold
War	1.0	fold
Conflict	1.0	fold
Cooperation	1.0	fold
Competition	1.0	fold
Collaboration	1.0	fold
Partnership	1.0	fold
Relationship	1.0	fold
Community	1.0	fold
Society	1.0	fold
Culture	1.0	fold
Religion	1.0	fold
Philosophy	1.0	fold
Art	1.0	fold
Literature	1.0	fold
Science	1.0	fold
Technology	1.0	fold
Industry	1.0	fold
Commerce	1.0	fold
Finance	1.0	fold
Health	1.0	fold
Education	1.0	fold
Government	1.0	fold
Law	1.0	fold
Justice	1.0	fold

5

10

15

39

APPENDIX 3

Program for Determining Strength of Wavelength Response in a Region

5

```
#include
<stdio.h>
#include
<stdlib.h>
#include
<math.h>

#define NMAX
3501
#define STRMAX
151
#define FNMAX
81
#define OUTPTS
801

void locate(float xx[], unsigned long n, float x,
unsigned long *j);
void norm(float xx[], unsigned long
int n);
void baseline(float xx[], unsigned
long int n);
void partinteg(float xx[], unsigned long int x1, unsigned long int
x2,
float *area);

int
main()
{
    char fnamein[FNMAX], string[STRMAX], *str_ptr,
fnameout[FNMAX], another;
    float xdata[NMAX], ydata[NMAX], xinter[OUTPTS+1],
yinter[OUTPTS+1];
    float
totalarea,aA,aB,aC,aD,aE,aF,aG,aH,aI,aJ,a
K;
    unsigned long int index, i,
j;
    int choice;
    FILE *fpin,
*fpout;
```

```
another = 'Y';
```

```
printf("Contact Rajdeep S. Kalgutkar, SRC-CRC 7-3003, for  
further info\n");
```

```
do {  
    for (i = 0; i <= NMAX-1;  
i++) {  
        xdata[i]=0;  
        ydata[i]=0;  
    };
```

```
    for (i = 0; i <= OUTPTS;  
i++) {  
        xinter[i]=0;  
        yinter[i]=0;  
    };
```

```
    printf("\nEnter name of the input file (80 chars max, no  
spaces): ");  
    scanf("%s",fnamein);
```

```
    printf("File name is  
%s\n",fnamein);
```

```
    fpin =  
fopen(fnamein,"r");
```

```
    if (fpin ==  
NULL) {  
        printf("Cannot open %s.  
Exiting...\n",fnamein);
```

```
exit(1);  
};
```

```
index = 1;
```

```
while (1) {  
    str_ptr = fgets(string,STRMAX-  
1,fpin);  
    if(str_ptr == NULL)  
        break;  
    if(index == NMAX)  
        break;  
    sscanf(string,"%f  
%f",&xdata[index],&ydata[index]);
```

```

        index++;
    };

    fclose(fpin);

    if((index == NMAX) && (str_ptr != NULL)) {
        index--;
        printf("Too many data points! Using first %d points
only...\n",index);
    }
    else {
        index--;
        printf("%d points
read...\n",index);
    };

    printf("\nEnter option for data
processing\n");
    printf("1: Simply interpolate the
data\n");
    printf("2: Normalize the data after
interpolation\n");
    printf("3: Baseline the data after
interpolation\n");
    printf("4: First interpolate, then baseline and finally
");
    printf("normalize the
data\n");
    printf("or\n");
    printf("0: to exit the program without any data
processing\n");
    printf("\nEnter option (0-
4): ");
    scanf("%d",&choice);

    if (choice == 0)

exit(2);

    printf("\nEnter name of the output file (80 chars max, no
spaces): ");
    scanf("%s",fnameout);

    printf("File name is
%s\n",fnameout);

    fpout =

```

```

fopen(fnameout,"w");

    if (fpout ==
NULL){
    printf("Cannot open %s.
Exiting...\n",fnameout);

exit(3);
    };

    for(i = 1; i <= OUTPTS;
i++) {
        xinter[i] = 200+((float)i-
1);
        locate(xdata,index,xinter[i],&j);
        if((j == 0) || (j ==
index))
            yinter[i] = 0;
        else
            yinter[i]=(xinter[i]-xdata[j])*((ydata[j+1]-
ydata[j])/
(xdata[j+1]-xdata[j]))+ydata[j];
    };

    if ((choice == 3) || (choice == 4)) {
baseline(yinter,OUTPTS);
    };

    if ((choice == 2) || (choice == 4)) {
        norm(yinter,OUTPTS);
    };

partinteg(yinter,51,OUTPTS,&totala
rea);

partinteg(yinter,51,101,&a
A);

partinteg(yinter,101,151,&
aB);

partinteg(yinter,151,201,&
aC);

```

```
partinteg(yinter,201,251,&
aD);
```

```
partinteg(yinter,251,301,&
aE);
```

```
partinteg(yinter,301,351,&
aF);
```

```
partinteg(yinter,351,401,&
aG);
```

```
partinteg(yinter,401,451,&
aH);
```

```
partinteg(yinter,451,501,&
aI);
```

```
partinteg(yinter,501,551,&
aJ);
```

```
partinteg(yinter,551,OUTPTS,&aK);
```

```
    fprintf(fpout,"The total area is:
%14.6E\n",totalarea);
    fprintf(fpout,"The area under region A is:
%6.2f%%\n",aA*100/totalarea);
    fprintf(fpout,"The area under region B is:
%6.2f%%\n",aB*100/totalarea);
    fprintf(fpout,"The area under region C is:
%6.2f%%\n",aC*100/totalarea);
    fprintf(fpout,"The area under region D is:
%6.2f%%\n",aD*100/totalarea);
    fprintf(fpout,"The area under region E is:
%6.2f%%\n",aE*100/totalarea);
    fprintf(fpout,"The area under region F is:
%6.2f%%\n",aF*100/totalarea);
    fprintf(fpout,"The area under region G is:
%6.2f%%\n",aG*100/totalarea);
    fprintf(fpout,"The area under region H is:
%6.2f%%\n",aH*100/totalarea);
    fprintf(fpout,"The area under region I is:
%6.2f%%\n",aI*100/totalarea);
    fprintf(fpout,"The area under region J is:
%6.2f%%\n",aJ*100/totalarea);
    fprintf(fpout,"The area under region K is:
%6.2f%%\n\n",aK*100/totalarea);
```

```

    for (i = 1; i <= OUTPTS-1; i++) {
        fprintf(fpout,"%13.5E, ",yinter[i]);
    };
    fprintf(fpout,"%13.5E\n",yinter[i]);

    fclose(fpout);

    printf("File %s
    written.\n\n",fnameout);
    printf("Process another file
    (Y/y/N/n)? : ");
    scanf("%1s",&another);
    } while (another == 'Y' || another
    == 'y');

    printf("Exiting...\n
    ");

    return(0
    );
    }

    void locate(float xx[], unsigned long n, float x,
    unsigned long *j)
    {
        unsigned long ju,jm,jl;
        int ascnd;

        jl=0;

        ju=n+1;
        ascnd=(xx[n] >= xx[1]);
        while (ju-jl > 1) {
            jm=(ju+jl) >> 1;
            if (x >= xx[jm] == ascnd)

        jl=jm;
        else

        ju=jm;
        }
        if (x == xx[1])
            *j=1;
        else if(x ==

```

```

xx[n])
    *j=n-
1;
    else
        *j=jl;
}

```

```

void norm(float xx[], unsigned long
int n)
{
    unsigned long
int i;
    float maxdata,
temp;

    maxdata =
xx[1];
    temp =
0;

    for(i = 2; i <= n; i++) {
        if(xx[i] >
maxdata)
            maxdata =
xx[i];
    };

    for(i = 1; i <= n; i++) {
        temp = xx[i]/maxdata;
        xx[i] = temp;
    };
}

```

```

void baseline(float xx[], unsigned
long int n)
{
    unsigned long
int i;
    float mindata,
temp;

    mindata = xx[1];
    temp =
0;

    for(i = 2; i <= n; i++) {
        if(xx[i] <

```

```

mindata)
    mindata =
xx[i];
};

```

```

for(i = 1; i <= n; i++) {
    temp = xx[i] - mindata;
    xx[i] = temp;
};
}

```

```

void partinteg(float xx[], unsigned long int x1, unsigned long int
x2,
    float *area)
{
    unsigned long
int i;
    float temp;

    temp =
0;

    for(i = x1; i <= x2 - 1; i++)
    {
        temp = temp + (xx[i] + xx[i+1])/2;
    };

    *area = temp;
}

```


APPENDIX 4

SRC Curing Resource dB 4 Query Select2

```
5 Sub Initialize
    Dim ses ses As New NotesSession
    Dim db_db As NotesDatabase
    Dim view view As NotesView
    Dim note _note1 As NotesDocument, note _note2 As NotesDocument
10 Dim i cnt As Integer, i add As Integer

Set db_db = ses ses.CurrentDatabase
Set note _note1 = ses ses.DocumentContext

15 Redim Preserve arr WavelengthRegion(0) air WavelengthRegion(0) _ ""

    If note _note1.Selection1(0) <> "" Or rwte _note1.Selection2(0) <> "" Then
        If note _note1.Selection1(0) <> "" Then
            Set view _view = db_db.GetView("By NoteID")
20
            If note _note1.Selection2(0) <> "" Then
                Set note _note2 = view _view.GetDocumentByKey(Right("00000000" &
                    note _note1.Selection2(0), 8))
            Else
25 Set note _note2 = view _view.GetDocumentByKey(Right("00000000" &
                    note _note1.Selection1(0), 8))
            End If

            If Not (note _note2 Is Nothing) Then
30 If note _note2.HasItem("WavelengthRegion") Then
                i_cnt = -1
                Forall vals In note _note2.WavelengthRegion
                    If vals <> "" Then
                        i_cnt = i_cnt + 1
35 Redim Preserve arr WavelengthRegion(i_cnt)
                        arr_WavelengthRegion(i cnt) = vals
                    End If
                End Forall

40 End If
End If End If

If note _note1.Type(0) = "S" Then
    Set view-view = db_db.GetView("Substrate")
45 Elseif note _note1.Type(0) = "P" Then
    Set view-view = db_db.GetView("InitiatorSensitizer") Else
    Set view-view = db_db.GetView("LightSource") End If
```

‘ Set note note2 =view-view. GetFirstDocument

i_cnt = -1

5 Do While Not (note note2 Is Nothing)

If note_note2.Name(0) <> "" Then

L add = True

If arr WavelengthRegion(0) <> "" Then

Ladd = False

10 Forall vals1 In note_note2.WavelengthRegion

Forall vals2 In arr_WavelengthRegion

If vals1 = vals2 Then

i_add = True

Exit Forall

15 End If

End Forall

If Ladd Then

Exit Forall

20 End If

End Forall

End If

If L add Then

25 i_cnt = i_cnt + 1

Redim Preserve arr_names(i_cnt)

arr_names(i_cnt) = note_note2.Name(0)

End If

End It

30

Set note note2 = view-view. GetNextDocument(note_note2)

Loop

note _notel .Names = arr_names

35 End Sub

SRC Curing Resource dB 4 Query Select2 Save Agent

Sub Initialize

40 Dim ses sesAs New NotesSession

Dim db_db As NotesDatabase

Dim view view As NotesView

Dim note_notel As NotesDocument, note_note2As NotesDocument

45 Set db_db = ses ses.CurrentDatabase

Set note note) = ses ses.DocumentContext

```

Select Case note_notel.Type(0)
Case "S"
Set view view = db_db.GetView("(Substrate)")

```

```

5 Set note_note2=view view.GetDocumentByKey(note_notel.Substrate(0))

```

```

Case "P"
Set view-view db-db.GetView("(InitiatorSensitizer)")

```

```

10 Set note_note2 -view view.GetDocumentByKey(note_notel.PhotolInitiator(O))

```

```

Case "L"
Set view-view =db db.GetView("(LightSource)")

```

```

15 Set note_note2 = view_view.GetDocumentByKey(note_notel.LightSource(0))

```

```

End Select

```

```

If note_notel.MexWction(0) = "Add" Then

```

```

20 If note_notel.Selection1(0) <> "" Then
Print "[!" + note_notel.dbname(O) + "/QuerySelection1?OpenForm&" &
note_notel.Selection1(0) & "&" & note_note2.Noteld & ")"

```

```

Else

```

```

25 Print "[!" + note_notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_note2.Noteld & "]"

```

```

End If Elseif note_notel.NextAction(O) = "Separate" Then

```

```

If note_notel.Selection1(0) <> "" Then

```

```

Print "[" + note_notel.dbname(O) + "/QuerySelection1?OpenForm&" &
note_notel.Selection1(O) & "&" & note_note2.Noteld & ")"

```

```

Else

```

```

30 Print "[!" + note_notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_note2.Noteld & ")"

```

```

End If

```

```

Elseif note_notel.NextAction(O) = "Separate" Then

```

```

35 If note_notel.Selection2(0) <> "" Then

```

```

Print "[" + note_notel.dbname(O) + "/QuerySelectionResults?OpenForm&" &
note_notel.Selection(0) & "&" & note_note2.Selection2(0) & _
"&" & note_note2.Noteld & "]"

```

```

Elseif note_notel.Selection1(0) <> "" Then

```

```

40 Print- "[" + note_notel.dbname(0) + "/QuerySelectionResults?OpenForm&" &
note_notel.Selection1(0) & "&" & note_note2.Noteld & ")"

```

```

Else

```

```

Print "[" + note_notel.dbname(O) + "lQuerySelectionResults?OpenForm&" &
note_noteMoteld & "]"

```

```

45 End If

```

```

Else

```

```

If note_notel.Selection2(0) <> "" Then

```

```

Print "[" + note_notel.dbname(0) + "/QuerySelectionOverlayResults?OpenForm&" &
note_notel.Selection1(0) & "&" & note_notel.Selection2(0) &
"&" & note_note2.Noteld & ")"
Elseif note_notel.Selection1(0) <> "" Then
5 Print "[" + note_notel.dbname(0) + "/QuerySelectionOverlayResults?OpenForm&"
& note_notel.Selection(0) & "&" & note_note2.Noteld & ")"
Else
Print "[" + note_notel.dbname(0) + "lQuerySelectionOverlayResults?OpenForm&"
& note_note2.Noteld & ")"
10 End If
End If
End Sub

```

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SRC Curing Resource dB 4 Query Overlay Open Agent

Sub Initialize

```

5      pim ses_ses As New NotesSession
      Dim db_db As NotesDatabase
      Dim view-view As NotesView
      Dim note_notel As NotesDocument, note_note2As NotesDocument
      Dim i_cntAs Integer, i_addAs Integer

10     Set db_db = ses ses.CurrentDatabase
      Set note_notel =ses ses.DocumentContext

      S et view-view = db_db. G etView("By N otel D ")

15     If note_notel.Selection1(0) <> "" Then
      S et note-note2 = view-view. G etD ocumentByKey(R ight("00000000" + note_note2.
      S election"! (0). 8))

20     If Not (note_note2 Is Nothing) Then
          note_notel.data1 = note_note2.EmissData
          note_notel.maxfreq1 = note_note2.MaxFreq
      End If End If

25     If note_note2.Selection2(0) <> "" Then
      Set note-note2 = view view.GetDocumentByKey(Right("00000000" +
      note_note2.Selection2(0), 8))

30     If Not (note_note2 Is Nothing) Then
          note_notel.data2=note_note2.EmissData
          note_notel.maxfreq2 = note_note2.MaxFreq
      End If End If

      If note_notel.Selection3(0) <> "" Then
35     Set note-note2 = view_view.GetDocumentByKey(Right("00000000" +
      note_note2.Selection3(0), 8))

      If Not (note_note2Is Nothing) Then
40         note_notel.data3 = note_note2.EmissData
          note_notel.maxfreq3=note_note2.MaxFreq
      End If End If End Sub

```

APPENDIX 5

```
import java.awt.*; import java.awt.event.*; import java.applet.*;
```

```
5 public class SRC Charts extends Applet { int gi count;
```

```
double GetHMax(String str_in) { String str_current; double dbl hmax;
```

```
10 str_current = ""; dblhmax = 0; for Tint i cnt = 0; i_cnt < str_in.length(); i cnt++) {  
if(str in. region Match es(i cnt, ",", 0, 2))  
if(Double.valueOf(str current).doubleValue() > dbl_hmax)  
dbl hmax = Double.valueOf(str current).doubleValue();  
str current = "" ;  
i_cnt++;  
15 gi count++; ) else {  
str current = str current.concat(str in.substring(i cnt, i cnt + 1));  
  
)  
if(str_current.length() > 0) {  
20 if(Double.valueOf(str_current).doubleValue() > dbl_hmax)  
dbl hmax = Double.valueOf(str_current).doubleValue(); gi count++; ) return dbl hmax;
```

```
int StringTolnt(String str_in, double dbl hmax) { double dbl_pos;
```

```
25 dbl_pos = getSize().height - (25 + (Double.valueOf(str_in).doubleValue() *  
((getSize().height - 50) / dbl hmax))); return (int)dbl-pos; )
```

```
30 void drawChartLine(Graphics g, String str_in, String str_type, double dbl_maxfreq) {  
double dbl_x, dbl_inc, dbl_hmax; String str last, str next;
```

```
str last str_next = "" ; dbl x = 25; gi count = 0;
```

```
35 dbl_hmax = GetHMax(str_in); if(str type. equals IgnoreCase("S")) dbl hmax = 100;
```

```
dbl inc = (((double)getSize().width - 50) / gi count) * ((dbl maxfreq - 200) / 800));
```

```

for (int i cnt = 0; i_cnt < str_in.length(); ) “, “, i c{
    nt++)if(str_in.regionMatches(i cnt, 0,
5    2))if(str_last.length(> 0)    {
        {
        g.drawLine((int)dbl x, StringToInt(str_last, dbl hmax), (int)(dbl x + dbl inc),
        StringToInt(str_next, dbl hmax));
        dbl x = dbl x + dbl inc;

10    str last = str_next; str next = “”; i cnt++;

    else { str next = str next.concat(str in.substring(i cnt, i cnt + 1));

    )
15    if(str_next.length() > 0)
        g.drawLine((int)dbl x, StringToInt(str_last, dbl hmax), (int)(dbl x + dbl-inc),
        StringToInt(strnext, dbl_hmax)); )

    public void paint(Graphics g) { double dbl x, dbl-y;

20    g.setColor(Color.black); g.drawLine(0, 0, getSize().width, 0); g.drawLine(25,
        getSize().height - 25, getSize().width - 25, getSize().height - 25); g.drawLine(25, 25,
        25, getSize().height - 25);

25    for(int i cnt = 0; i_cnt < 9; i cnt++) {
        dbl_x = 25 + (((double)i cnt * (((double)getSize().width - 50) / 8));
        g.drawLine((int)dbl x, getSize().height - 25, (int)dbl x, getSize().height - 20);
        g.drawString(String.valueOf((i cnt * 100) + 200), (int)dbl x - 8, getSize().height - 5); )

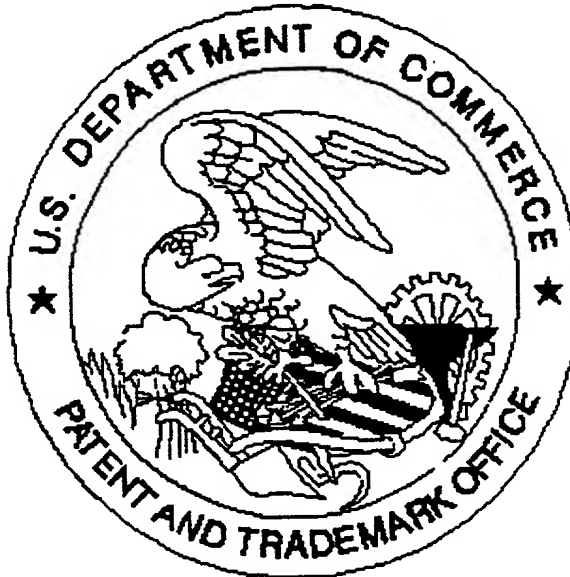
30    for(int i cnt = 0; i_cnt < 11; i_cnt++) {
        dbl-y = 25 + (((double)i cnt * (((double)getSize().height - 50) / 10));
        g.drawLine(20, (int)dbl-y, 25, (int)dbl-y);
        g.drawString(String.valueOf(100 - (i cnt * 10)), 1, (int)dbl-y + 5); )

35    g.drawString(“Data Overlay”, (getSize().width / 2) - 30, 12);

    g.setColor(Color.red); drawChartLine(g, getParameter(“Data 1 “), getParameter(“Type
    1 “), Double.valueOf(getParameter(“Max Freq 1 “)).doubleValue());
    g.setColor(Color.blue); drawChartLine(g, getParameter(“Data 2”),
40    getParameter(“Type 2”), Double.valueOf(getParameter(“Max Freq
    2”)).doubleValue()); g.setColor(Color.green); drawChartLine(g, getParameter(“Data
    3”), getParameter(“Type 3”), Double.valueOf(getParameter(“Max Freq
    3”)).doubleValue()); ) )

```

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